

Optimal linear Kawasaki model

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Abstract. The Kawasaki model is not exactly solvable as any choice of the exchange rate ($w_{jj'}$) which satisfies the detailed balance condition is highly nonlinear. In this work we address the issue of writing $w_{jj'}$ in a best possible linear form such that the mean squared error in satisfying the detailed balance condition is least. In the continuum limit, our approach leads to a Cahn-Hilliard equation of conservative dynamics. The work presented in this paper will help us anticipate how the conservative dynamics of an arbitrary Ising system depends on the temperature and the coupling constants. In particular, for two and three dimensional systems, the critical temperatures estimated in our work are in good agreement with the actual values. We also calculate the dynamic and some of the critical exponents of the model.

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1. Introduction

From an arbitrary given state how does a system relax to its equilibrium state? Answering this question remains one of the major challenges in theoretical physics. Even after a century of rigorous research, our understanding of nonequilibrium systems is modest. Though we have a well defined prescription to address any issue regarding an equilibrium state, we are yet to develop a general framework to study some irreversible process. In this challenging situation, it is important to study the simple physical models in order to gain some insight into the nonequilibrium processes.

The Ising model is one of the simplest non-trivial models to study the underlying physics of many irreversible processes. Here the main two microscopic mechanisms, by which a system equilibrates, are due to Roy J. Glauber [1] and K. Kawasaki [2]. While the first mechanism (Glauber's) describes a non-conservative order-parameter dynamics, the second one is thought to be the underlying mechanism for a conservative order-parameter dynamics. The Glauber dynamics is exactly solvable only for one dimensional Ising system, on the other hand, the Kawasaki dynamics is not exactly solvable even for one dimensional system. Though the choice of transition rate or exchange rate

for the two kinetic models are not unique, it has to be such that the detailed balance condition at equilibrium is satisfied. Although it is possible to get some nonlinear form of the transition rate or exchange rate for which the detailed balance condition is satisfied, unfortunately, the kinetic models are not exactly solvable with this nonlinear form (except for the aforementioned case).

It has been a real challenge to study analytically these two kinetic models for an arbitrary Ising system (in any dimension) without compromising on the detailed balance condition. Recently one of us (with another author) developed a general mathematical method to study the Glauber dynamics in an arbitrary Ising system [3]. It may be noted that, the linear Glauber model, where the chosen transition rate is linear, is exactly solvable although the detailed balance condition is not exactly satisfied [4, 5, 6]. In our mathematical approach [3], a linear form of the transition rate with an appropriate number of parameters is taken. These parameters are then optimized in such a way that the mean squared error in satisfying the detailed balance condition is least. The advantage of this method is that, it helps us to anticipate how the kinetic properties of an Ising system depend on the temperature and coupling constant. Along with many other things, it was shown in that work that, using the method it is possible to derive a time-dependent Ginzburg-Landau equation (linear version) for the non-conservative dynamics from the Glauber's microscopic model [3]. In this paper, we use this optimal linearization approach to study the Kawasaki dynamics in an arbitrary Ising model. It will be shown here how a Cahn-Hilliard equation (linear version) for the conservative dynamics can be derived from the Kawasaki's microscopic model. It is very encouraging to find that the critical temperatures (for two and three dimensional systems) estimated from the divergence of the correlation length or the critical slow down are in very good agreement with the actual values. We also calculate the dynamic exponent and some of the critical exponents for our optimal linear model.

Our paper is organized in the following way. In section 2, we give a detailed description of our approach. In the next section (sec 3), we apply our method to study Ising systems in different dimensions. We conclude our work in section 4.

2. General theory

Let us consider an Ising system of N interacting spins ($\sigma_i = \pm 1$). For simplicity, we will consider in this work a uniform (or isotropic) ferromagnetic system where all the coupling constants are same. It will be also assumed that there is only nearest neighbor interactions and the system is on a hyper-cubic lattice. The relevant Hamiltonian is given by,

$$H = -J \sum_{\langle jj' \rangle} \sigma_j \sigma_{j'}, \quad (1)$$

where J is the coupling constant (> 0). We further consider that $p(\{\sigma\}; t)$ is the probability that the spins take the values $\sigma_1, \dots, \sigma_N$ at time t . A master equation for

the time evolution of the probability is given by,

$$\frac{d}{dt}p(\{\sigma\};t) = - \sum_{\langle jj' \rangle} w_{jj'}(\sigma_j \sigma_{j'}) p(\{\sigma\};t) + \sum_{\langle jj' \rangle} w_{jj'}(\sigma_{j'} \sigma_j) p(\{\sigma\}_{jj'};t), \quad (2)$$

where summations run over all possible nearest neighbor pairs. $\{\sigma\}_{jj'}$ represents the same state as $\{\sigma\}$ with spins of the pair jj' exchanged (i.e., $\sigma_j \rightarrow \sigma_{j'}$ and $\sigma_{j'} \rightarrow \sigma_j$). In Kawasaki dynamics, the exchange rate $w_{jj'}(\sigma_j \sigma_{j'})$ for the neighboring pair jj' is the transition rate from the state $\{\sigma\}$ to the state $\{\sigma\}_{jj'}$.

By considering $\sigma_j(t)$ as stochastic function of time, we consider two important quantities, namely, a time dependent average spin value $q_j(t)$ and a time dependent correlation function $r_{i,j}(t)$. These are given below,

$$q_j(t) = \langle \sigma_j(t) \rangle = \sum_{C(N)} \sigma_j p(\{\sigma\};t) \quad (3)$$

$$r_{i,j}(t) = \langle \sigma_i(t) \sigma_j(t) \rangle = \sum_{C(N)} \sigma_i \sigma_j p(\{\sigma\};t). \quad (4)$$

Here summation is over all possible (2^N in number) spin configurations, $C(N)$. It may be noted that $r_{j,j} = 1$.

We now write time derivative of these quantities as first step to obtain them as function of time. It is easy to get the derivatives of q_j and $r_{i,j}$ by multiplying respectively σ_k and $\sigma_j \sigma_k$ to Eq. (2) and then sum them over all possible spin configurations. Some easy manipulations would give us the following equations:

$$\frac{d}{dt}q_k(t) = -2 \sum_{C(N)} \sum_{k'=L_k} \sigma_k w_{kk'}(\sigma_k \sigma_{k'}) p(\{\sigma\};t) \quad (5)$$

$$\begin{aligned} \frac{d}{dt}r_{j,k}(t) = -2 \sum_{C(N)} \sigma_j \sigma_k \left\{ \sum_{j'=L_j} w_{jj'}(\sigma_j \sigma_{j'}) \right. \\ \left. + \sum_{k'=L_k} w_{kk'}(\sigma_k \sigma_{k'}) \right\} p(\{\sigma\};t). \end{aligned} \quad (6)$$

Here, for example, the second summation in Eq. (5) is over all neighbors of the k th site (denoted by L_k).

To solve these equations, a choice of $w_{jj'}$ has to be made. The exchange rate $w_{jj'}$ should be chosen in such a way that it satisfies the equation of detailed balance (EDB) at the equilibrium. In addition, it should be zero when neighboring pairs jj' are both up or both down. We here use Suzuki-Kubo form for $w_{jj'}$ which satisfies the EDB at equilibrium [9, 10]. To make sure that the rate is zero when both the spins are aligned along the same direction, we multiply $w_{jj'}$ by a factor $\frac{1}{2}(1 - \sigma_j \sigma_{j'})$. So our chosen form for $w_{jj'}$ is given by,

$$w_{jj'}(\sigma_j \sigma_{j'}) = \frac{\alpha}{2} \left[1 - \tanh \left(\frac{\beta \Delta E}{2} \right) \right] \cdot \frac{1}{2} (1 - \sigma_j \sigma_{j'}), \quad (7)$$

with ΔE being the energy difference between the final state $\{\sigma\}_{jj'}$ and the initial state $\{\sigma\}$. Here β is the inverse temperature $1/(k_B T)$ with k_B being the Boltzmann constant.

The parameter α sets the timescale of the nonequilibrium process. It is not difficult to see that,

$$\Delta E = J(\sigma_j - \sigma_{j'}) \left(\sum'_{m=L_j} \sigma_m - \sum'_{n=L_{j'}} \sigma_n \right). \quad (8)$$

Here the first (second) primed summation runs over all the neighbors of j th (j' th) site excluding the j' th (j th) site. Now using the above expression of ΔE in Eq. (7), we get,

$$w_{jj'}(\sigma_j \sigma_{j'}) = \frac{\alpha}{2} \left[\frac{1}{2}(1 - \sigma_j \sigma_{j'}) - \frac{1}{2}(\sigma_j - \sigma_{j'}) \tanh \left\{ \beta J \left(\sum'_{m=L_j} \sigma_m - \sum'_{n=L_{j'}} \sigma_n \right) \right\} \right]. \quad (9)$$

Unfortunately, this exact nonlinear form of $w_{jj'}$ is intractable for the analytical study of dynamics. A linear form of $w_{jj'}$ is easy to handle, but, generally it does not exactly satisfy the detailed balance condition. We now present a mathematical approach to linearize $w_{jj'}$ in such a way that the mean squared error in satisfying the detailed balance condition is least.

2.1. Linearization of $w_{jj'}$ using a least squares method

In this subsection we will see how one can linearize the Suzuki-Kubo form of the exchange rate in an optimal way. More specifically, we will discuss here the best possible way to linearize hyperbolic-tan function appearing in $w_{jj'}$; this will in turn ensure that, the error in satisfying the EDB is least [3]. The remaining nonlinearity in $w_{jj'}$ due to the constraint term $\frac{1}{2}(1 - \sigma_j \sigma_{j'})$ will be systematically handled in section 3.

Let us consider a hyperbolic-tan function of Ising variables $\tanh [\sum_k p_k \sigma_k]$, where p_k are some dimensionless real parameters. Noting the series $\tanh x = x - \frac{x^3}{3} + \dots$, we can attempt to linearize our hyperbolic-tan function by considering,

$$\tanh \left[\sum_{k=1}^L p_k \sigma_k \right] \approx \sum_{k=1}^L \gamma_k \sigma_k. \quad (10)$$

Here the coefficients γ_k 's are not just p_k 's that appear in the first order term of the hyperbolic-tan series. These coefficients also have contributions from the higher order terms of the series (this will be clear by noting that, $\sigma_j^m = 1$ if m is even and $\sigma_j^m = \sigma_j$ if m is odd). Although by analyzing the series it is possible to find out the exact values of γ_k 's, it is best to take the optimal values for the γ_k 's which can be obtained by a linear regression process. By taking the optimal values, we ensure that the error introduced due to linearization is minimum. The optimization process somewhat compensates the absence of the nonlinear terms in our desired linear form of w_j (nonlinear terms are typically product of different σ 's).

To do a linear regression, we will consider γ_k 's in Eq. (10) as the parameters of the regression process. We may note that, Eq. (10) actually represents 2^L linear

equations in L parameters. Each of these linear equations corresponds to the one of the 2^L configurations of the L Ising variables. Obviously, no set of values for the γ 's can simultaneously satisfy the overdetermined set of 2^L linear equations. We will now see how the best possible values for γ 's, for which mean squared error is minimum, can be obtained.

Before discussing the linear regression process, it may be worth mentioning here that, the function $\tanh x$ is linear about the origin ($x = 0$). Since the term $[\sum_{k=1}^L p_k \sigma_k]$ is zero or close to zero for a good fraction of the total number of configurations (at least for isotropic case when p_k 's are equal), we expect our linearization to work reasonably good in a normal situation.

When all p_k 's are different, we need to consider L number of independent parameters (γ 's). A Moore-Penrose pseudoinverse matrix of dimension $L \times 2^L$ can be used to get the best possible values of the parameters (γ 's). This pseudoinverse matrix involved in the regression process is obtained solely from the configuration matrix (whose different rows represent different configurations of the L Ising spins) and does not depend on any parameter of the problem. A general discussion on this topic can be found in Ref. [3]. We will consider a special case here. Since our system is isotropic (all the coupling constants are same) with only nearest neighbor interactions, values of all the parameters obtained in the regression process will be effectively same. Therefore consideration of a single parameter in the regression process is good enough for the present purpose; let this parameter be γ . The regression process is now reduced to finding the best possible value of the parameter from the following set of equations:

$$\tanh \left\{ \beta J \left(\sum'_{m=L_j} \sigma_m - \sum'_{n=L_{j'}} \sigma_n \right) \right\} \approx \gamma \left(\sum'_{m=L_j} \sigma_m - \sum'_{n=L_{j'}} \sigma_n \right). \quad (11)$$

If L be the number of Ising variables involved in the above expression, we may note that the above expression actually represents 2^L equations corresponding to each of that many configurations. Here, if z is the coordination number or the number of nearest neighbors (2, 4, and 6 respectively for one, two and three dimensional systems), then $L = 2(z - 1)$. In the regression process, the left side of Eq. (11) will be represented by a column matrix with 2^L elements; let us denote this column by Ω . Similarly, the quantity inside the bracket in the right side of Eq. (11) will again be represented by a column matrix with 2^L elements; we will denote this column by C matrix. An error function can now be defined from these two column matrices: $S(\gamma) = \sum_{i=1}^{2^L} |\Omega_i - \gamma C_i|^2 = \|\Omega - \gamma C\|^2$. The best possible value of the parameter γ can be obtained by minimizing the error function $S(\gamma)$. The formal solution for γ can be written using the Moore-Penrose pseudoinverse matrix $C^+ = (C^T C)^{-1} C^T$, which in the present case is just a row matrix with 2^L number of elements. The solution is given by the following relation:

$$\gamma = C^+ \Omega. \quad (12)$$

To get the exact expression of γ in terms of the parameters β and J , we note that, among the 2^L number of elements of the column matrix C , one element will be L and,

due to Z_2 symmetry, $-L$ will be another element. There will be ${}^L C_1$ number of elements with the value $L-2$ and equal number of elements with the value $-L+2$. This counting goes on till we get ${}^L C_{\frac{L}{2}}$ number of 0's (note, L is always even). For us $C^T C$ is just a number whose value is $L2^L$. The pseudoinverse matrix in the present case is given by, $C^+ = \frac{2^{-L}}{L} C^T$. We notice that if i th element of the C matrix is, say, Y , then the i th element of the Ω matrix will be $\tanh(\beta J Y)$. Now using Eq. (12), it is easy to get the desired expression for the γ :

$$\gamma = \frac{2^{-L+1}}{L} \sum_{i=1}^{L/2} Z_i {}^L C_{i-1} \tanh[\beta J Z_i], \quad (13)$$

where $Z_i = L - 2i + 2$ (here we again remember that $L = 2(z - 1)$).

Using this optimal linearization of hyperbolic-tan function, we can rewrite the exchange rate give in Eq. (9) as,

$$w_{jj'}(\sigma_j \sigma_{j'}) = \frac{\alpha}{4} \left[(1 - \sigma_j \sigma_{j'}) - \gamma(\sigma_j - \sigma_{j'}) \left(\sum'_{m=L_j} \sigma_m - \sum'_{n=L_{j'}} \sigma_n \right) \right]. \quad (14)$$

It may be worth commenting here about the nature of the steady state that one would get by using the above exchange rate. We may note that, to satisfy the detailed balance condition, the local probability current for any pair jj' , $I_{jj'} = -w_{jj'}(\sigma_j \sigma_{j'}) p(\{\sigma\}) + w_{jj'}(\sigma_{j'} \sigma_j) p(\{\sigma\}_{jj'})$, should be zero for every configuration of its neighbours (here $p(\{\sigma\})$ is the Maxwell-Boltzmann probability factor defined for the configuration $\{\sigma\}$). Had we taken the nonlinear form for $w_{jj'}$, as given in Eq. (9), the current $I_{jj'}$ would have been zero for the every configuration of its neighbours. With the exchange rate given in Eq. (14), the current will not be zero for every configurations -sometimes it will be positive and sometimes negative. In this context, as explained in Ref. [3], our method ensures following things: (a) the average local probability current $\langle I_{jj'} \rangle$ (average over all possible configurations of neighbors) is zero, and (b) two opposite tendencies (forward currents and backward currents depending on the sign of $I_{jj'}$) are individually as low as possible on the average.

3. Study of dynamics in continuum limit

A continuum approach will be adopted in this section to study the Kawasaki dynamics. We will see that in this limit both the equation for the average local spin and the equation for the correlation function (see Eqs. (5) and (6)) take the same form with parameters of the equations differ only by a factor of 2.

3.1. Equation for local magnetization

We will first consider the one dimensional system. Using the exchange rate from Eq. (14), we get from Eq. (5):

$$\frac{d}{dt} q_k(t) = -\frac{\alpha}{2} [(2q_k - q_{k-1} - q_{k+1})$$

$$\begin{aligned}
& -\gamma (q_{k+1} + q_{k-1} - q_{k+2} - q_{k-2}) \\
& -\gamma (-2 < \sigma_{k-1} \sigma_k \sigma_{k+1} > + < \sigma_{k-2} \sigma_{k-1} \sigma_k > + < \sigma_k \sigma_{k+1} \sigma_{k+2} >) \}. \quad (15)
\end{aligned}$$

Now in the continuum limit if $Q(x, t)$ denotes the local magnetization at the location x and time t , then the first group of terms in the right hand side, i.e. $2q_k - q_{k-1} - q_{k+1}$, can be recognized as $-\frac{d^2}{dx^2}Q(x, t)$. Similarly, the second group of terms, i.e. $q_{k+1} + q_{k-1} - q_{k+2} - q_{k-2}$, can be recognized as $-3\frac{d^2}{dx^2}Q(x, t)$. Last or third group of terms, where all the terms are three-point correlation functions, is difficult to deal with. To make the calculations tractable, we will replace the nonlinear terms like $\sigma_{k-1}\sigma_k\sigma_{k+1}$ by a suitable linear form. Let us consider that the Ising system is momentarily fixed (say, at time t). This ‘frozen’ system will have domains of ‘up’ and ‘down’ spins. We now note here that, when all the three spins, i.e. $(k-1)$ th, k th and $(k+1)$ th spins, are from the same domain, they will be aligned along the same direction. The value of the product of these spins will be same as the value of a single spin. That is to say, $\sigma_{k-1}\sigma_k\sigma_{k+1} = \sigma_k$ if all the three spins are from the same domain. If $(k-1)$ th and k th spins are from one domain and $(k+1)$ th spin is from the next domain, then the above linearization will not work. Similarly, this linearization also breaks down when $(k-1)$ th spin is in one domain and the other two spins are from the next domain. This indicates that we need to consider one more term whose value is zero inside a domain and which appropriately adjusts the boundary effects. A careful inspection shows that the term $(\sigma_{k-1} - 2\sigma_k + \sigma_{k+1})$ fulfils our requirement. So we replace $\sigma_{k-1}\sigma_k\sigma_{k+1}$ by the following linear term: $\sigma_k + (\sigma_{k-1} - 2\sigma_k + \sigma_{k+1})$. This linearization will not only be valid inside a domain but also at boundaries. More specifically, above linearization is exact for the following four configurations: $(1,1,1)$, $(-1,-1,-1)$, $(1,1,-1)$ and $(-1,-1,1)$. Here it should be also mentioned that this linearization does not work for an isolated spin in a domain (like an up spin inside a down spin domain), i.e., it fails for the remaining two configurations $(1,-1,1)$ and $(-1,1,-1)$. However it can be safely assumed that, after some time in the coarsening, the number of such isolated spins becomes extremely small compared to the total number of spins N (which is assumed to be thermodynamically large). Here we may recall that in a spin exchange dynamics there is zero chance that a spin inside a domain will suddenly flip to become such an isolated spin. Above argument shows that the error introduced due to the linearization of the three-point correlation function can be assumed to be very small. In the continuum limit, if we denote $< \sigma_{k-1}\sigma_k\sigma_{k+1} >$ by $S(x, t)$, then the linearization allows us to write $S(x, t) = Q(x, t) + \frac{d^2}{dx^2}Q(x, t)$. The third group of terms in the right hand side of Eq. (15) can now be written as $\frac{d^2}{dx^2}S(x, t)$ or, $\frac{d^2}{dx^2}Q(x, t) + \frac{d^4}{dx^4}Q(x, t)$.

With the continuum limit representation of all the terms in Eq. (15), we now write the equation for the local magnetization in the continuum limit:

$$\frac{\partial}{\partial t}Q(x, t) = \frac{\alpha}{2}(1 - 2\gamma)\frac{d^2}{dx^2}Q(x, t) - \frac{\alpha}{2}\gamma\frac{d^4}{dx^4}Q(x, t). \quad (16)$$

Using the same line of arguments, it is possible to generalize this equation to the

higher dimensions. In dimension d , the equation reads in the following way,

$$\frac{\partial}{\partial t}Q(\vec{r}, t) = D\nabla^2Q(\vec{r}, t) - \kappa\nabla^4Q(\vec{r}, t). \quad (17)$$

Here $Q(\vec{r}, t)$ is the local magnetization at the location \vec{r} and time t . In the above equation, the diffusion constant $D = \frac{\alpha}{2}(1 - 2d\gamma)$ and the bidiffusion constant $\kappa = \frac{\alpha}{2}\gamma$. The term d represents the dimensionality of the system (i.e., $d = 1, 2$ or 3 for one, two or three dimensional system respectively). The parameter γ depends on dimensionality d ($=z/2$) and is given by Eq. (13).

After adopting all these linearization approximations, one would like to know if the dynamics still remains conservative. It is in fact very easy to check from Eq. (15). After replacing three point correlation terms by their appropriate linear versions, if we sum the terms of Eq. (15) over all the sites, we will get $\frac{dM(t)}{dt} = 0$, where $M(t)$ is the total magnetization ($= \sum_{k=1}^N q_k$). This shows that $M(t)$ remains constant over time as expected for a conservative dynamics. This fact can also be explicitly checked for higher dimensional systems.

Eq. (17) is in the form of the well known Cahn-Hilliard equation (linear version) of the conservative dynamics [11, 12], which has been subject of active study for the last few decades [7, 8, 10]. The work presented in this paper thus establishes a connection between the phenomenological Cahn-Hilliard theory and the Kawasaki's microscopic model for conservative dynamics. Advantage of the present work is obvious; it gives us explicit temperature and exchange constant dependence of the parameters involved in the Cahn-Hilliard equation. For two and three dimensional systems, the critical temperatures estimated by analyzing this equation are in very good agreement with the well know actual values (section 3.3). Here it may be further added that, if the equation for a non-conservative order parameter Q is of the form $\frac{\partial}{\partial t}Q = F(Q)$, then the corresponding equation for the case where Q is a conserved order parameter is given by: $\frac{\partial}{\partial t}Q = -\nabla^2F(Q)$ [7]. In this respect, Eq. (17) is consistent with the time-dependent Ginzburg-Landau equation derived from the Glauber's model in our previous work [3] within the same optimal linearization approximation.

3.2. Equation for two-point correlation

Similar to the treatment of the local magnetization, we will first consider here the one dimensional system. Using the exchange rate from Eq. (14), we get from Eq. (6):

$$\begin{aligned} \frac{d}{dt}r_{j,i}(t) = & -\alpha [(2r_{j,i} - r_{j,i-1} - r_{j,i+1}) \\ & -\gamma (r_{j,i+1} + r_{j,i-1} - r_{j,i+2} - r_{j,i-2}) \\ & -\gamma (-2 < \sigma_j \sigma_{i-1} \sigma_i \sigma_{i+1} > + < \sigma_j \sigma_{i-2} \sigma_{i-1} \sigma_i > + < \sigma_j \sigma_i \sigma_{i+1} \sigma_{i+2} >)] \end{aligned} \quad (18)$$

Now in the continuum limit if $G(x, t)$ denotes the time dependent correlation between two spins separated by a distance x ($x = |i - j|$), then the first group of terms, i.e. $2r_{j,i} - r_{j,i-1} - r_{j,i+1}$, can be recognized as $-\frac{d^2}{dx^2}G(x, t)$. Similarly, the second group of terms can be recognized as $-3\frac{d^2}{dx^2}G(x, t)$. Last or third group of terms, where

all the terms are four point correlation functions, is again difficult to deal with. If we now adopt the linearization discussed in the last subsection, i.e., if we replace the terms like $\sigma_{i-1}\sigma_i\sigma_{i+1}$ by the terms like $\sigma_i + (\sigma_{i-1} - 2\sigma_i + \sigma_{i+1})$, then the third term in Eq. (18) can be recognized as $\frac{d^2}{dx^2}G(x, t) + \frac{d^4}{dx^4}G(x, t)$. This enables us to write the equation for the correlation function in the following way:

$$\frac{\partial}{\partial t}G(x, t) = \alpha(1 - 2\gamma)\frac{d^2}{dx^2}G(x, t) - \alpha\gamma\frac{d^4}{dx^4}G(x, t). \quad (19)$$

It is again straightforward to generalize this equation for the higher dimensional systems. The result is given below,

$$\frac{\partial}{\partial t}G(r, t) = 2D\nabla^2G(r, t) - 2\kappa\nabla^4G(r, t). \quad (20)$$

Here $G(r, t)$ is the correlation function between the sites separated by a distance r ($= |\vec{r}|$). In the equation, we have again $D = \frac{\alpha}{2}(1 - 2d\gamma)$ and $\kappa = \frac{\alpha}{2}\gamma$. Physically appealing general solution of this equation is difficult. We will only consider its steady state solution in section 3.4.

3.3. Dynamical exponent, correlation length and critical temperature

To gain some insight into Eq. (17), we will do a Fourier analysis of the equation. This analysis will give us the equation for each mode \vec{k} :

$$\frac{\partial Q(\vec{k}, t)}{\partial t} = -k^2(D + \kappa k^2)Q(\vec{k}, t), \quad (21)$$

Solution of this equation gives, $Q(\vec{k}, t) = Q(\vec{k}, 0)e^{-t/\tau(\vec{k})}$, where the relaxation time for the mode \vec{k} is given by:

$$\tau(\vec{k})^{-1} = \kappa k^2(k^2 + \xi^{-2}). \quad (22)$$

Here the correlation length $\xi = \sqrt{\frac{\kappa}{D}} = \sqrt{\frac{\gamma}{1-2d\gamma}}$.

The dynamic exponent (denoted by z ; not to be confused with coordination number) is defined by how the maximum possible value of the relaxation time (τ_{\max}) scales with the system's relevant length scale. If we consider a finite but large system of size L , then $k_{\min} \sim 1/L$. Now when $k \ll \xi^{-1}$, then $\tau_{\max} \sim k_{\min}^{-2}\xi^2$, i.e., $\tau_{\max} \sim L^2\xi^2$. In this limit, both the length scales (L and ξ) are relevant; individually for both of them $z = 2$. In the other limit when the correlation length is of the order of L , then $\tau_{\max} \sim L^4$. In this case $z = 4$.

When the system approaches criticality, one expects the correlation length ξ to diverge. Using this fact, it is possible to estimate the critical temperature (T_C) which satisfies the following equation,

$$1 - 2d\gamma = 0. \quad (23)$$

For one dimensional system, $z = 2$ and accordingly $L = 2(z - 1) = 2$. Here $\gamma = \frac{1}{2}\tanh(2\beta J)$ (see Eq. (13)). In this case Eq. (23) takes the following form: $\tanh(2\beta J) = 1$. This will be only satisfied when $\beta \rightarrow \infty$. Therefore in this case

$T_C = 0$, in accordance with the fact that the one dimensional Ising system behaves critically only near to absolute zero temperature.

For two dimensional system (square lattice), $z = 4$ and accordingly $L = 6$. Here $\gamma = \frac{1}{32}[\tanh(6\beta J) + 4\tanh(4\beta J) + 5\tanh(2\beta J)]$ (see Eq. (13)). In this case Eq. (23) takes the following form: $\tanh(6\beta J) + 4\tanh(4\beta J) + 5\tanh(2\beta J) = 8$. Solution of this equation gives $T_C = 2.493J/k_B$, whereas its exact value is known to be $T_C = 2.269J/k_B$ [13].

For three dimensional system (simple cubic lattice), $z = 6$ and accordingly $L = 10$. Here $\gamma = \frac{1}{512}[\tanh(10\beta J) + 8\tanh(8\beta J) + 27\tanh(6\beta J) + 48\tanh(4\beta J) + 42\tanh(2\beta J)]$ (see Eq. (13)). In this case Eq. (23) takes the following form: $[\tanh(10\beta J) + 8\tanh(8\beta J) + 27\tanh(6\beta J) + 48\tanh(4\beta J) + 42\tanh(2\beta J)] = 256/3$. Solution of this equation gives $T_C = 4.342J/k_B$, whereas its actual value is expected to be about $T_C = 4.511J/k_B$ [14, 15, 16].

We see here that the values of the critical temperatures (T_C) are in very good agreement with the actual ones, and an impressive improvement over the mean field values (where $T_C = zJ/k_B$ with $z = 2, 4$ and 6 for one, two and three dimensional systems respectively). It is here encouraging to notice that our approach correctly captures the basic physics of the Ising model in different dimensions, viz., while the one dimensional system does not exhibit criticality at any finite temperature, the two and three dimensional systems do exhibit criticality at finite temperatures.

Before finishing this subsection, we briefly comment on scaling behavior of the correlation length. Near to the criticality, the correlation length diverges as, $\xi \sim |\frac{T-T_C}{T_C}|^{-1/2}$ which can be seen by noting that $|1 - 2d\gamma| \sim |\frac{T-T_C}{T_C}|$. This shows that the critical exponent $\nu = 1/2$ (for $d = 2$ and 3).

3.4. Steady state correlation function

As we mentioned before, for a general case, physically appealing solution of Eq. (20) is difficult. It is though possible to quickly look into specific aspects of the equation, for example, by studying its steady state solution. If $P(r)$ is the function $G(r, t)$ for $t \rightarrow \infty$, then $P(r)$ should satisfy the following equation:

$$\nabla^2 P(r) = \xi^{-2} P(r), \quad (24)$$

where again the correlation length $\xi = \sqrt{\frac{\kappa}{D}} = \sqrt{\frac{\gamma}{1-2d\gamma}}$. The solution of this equation can be found in Ref. [3]. A trial solution of the form $\frac{e^{-r/\xi}}{r^l}$ can be taken to find the desired solution for $P(r)$. Here l is a constant to be determined; we find that $l = 0$ and 1 for $d = 1$ and 3 respectively. For $d = 2$, the above trial form does not yield any solution of Eq. (24). For this special case, we take the following trial form: $P(r) = S(r)e^{-r/\xi}$. It is easy to see that $S(r)$ satisfies the following equation:

$$\xi r \frac{d^2 S(r)}{dr^2} + (\xi - 2r) \frac{dS(r)}{dr} - S(r) = 0. \quad (25)$$

Solution of this equation can most easily be found by a trial series of the form $S(r) = \sum_{n=0}^{\infty} a_n r^n$. We obtain the following solution for the function: $S(r) =$

$a_0[1 + \sum_{n=1}^{\infty} \frac{(2n-1)!!}{(n!)^2} (r/\xi)^n]$. With this result, we now write down the solution for $P(r)$:

$$P(r) = a_0 e^{-r/\xi} \begin{cases} 1, & d = 1 \\ 1 + \sum_{n=1}^{\infty} \frac{(2n-1)!!}{(n!)^2} (r/\xi)^n, & d = 2 \\ \frac{1}{r}, & d = 3. \end{cases} \quad (26)$$

The value of a_0 can be determined by a normalization condition (the value will be, of course, different for different dimensions). Near to the criticality ($\xi \rightarrow \infty$), it is easy to see that $P(r) \sim \mathcal{O}(1)$, $\mathcal{O}(1)$ and $1/r$ for one, two and three dimension respectively (we assume here $r \ll \xi$). This suggests that the values of the critical exponent η , defined as $P(r) \sim r^{-(d-2+\eta)} e^{-r/\xi}$, are 1, 0 and 0 respectively for $d = 1, 2$ and 3.

3.5. Some additional remarks

We would like to make some comments here before finishing this section. The diffusion constant D (coefficient of the second order term in Eq. (17)) vanishes at criticality ($T = T_C$). This shows that the diffusion process goes through a critical slow down near T_C . We see that at the criticality, Eq. (17) reduces to a bidiffusion equation, $\frac{\partial}{\partial t} Q(\vec{r}, t) = -\kappa \nabla^4 Q(\vec{r}, t)$. It is easy to solve this equation, using Fourier transforms, and check that the average domain size grows as $L(t) \sim t^{1/4}$ [7]. By now it is though well established that $L(t) \sim t^{1/3}$ after a deep quench [7, 8]. This contradictory results may not be surprising as at the criticality, due to critical slow down, we expect slower growth rate of domains.

4. Conclusion

The Kawasaki model is not exactly solvable (in any dimension) as the exchange rate ($w_{jj'}$) involved in the calculations is highly nonlinear. To make the calculations tractable, in this paper we discussed a mathematical way to linearize $w_{jj'}$ in such a way that the mean squared error in satisfying the detailed balance condition is least. In the continuum limit, our approach leads to a Cahn-Hilliard equation of conservative dynamics. This establishes a connection between the phenomenological Cahn-Hilliard theory and the Kawasaki's microscopic model for conservative dynamics. Advantage of our work is that it will help us anticipate how the conservative dynamics of an arbitrary Ising system depends on the temperature and the coupling constants. In particular, the critical temperatures estimated from the divergence of correlation length or the critical slow down are in very good agreement with the actual values.

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